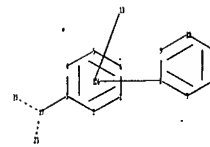
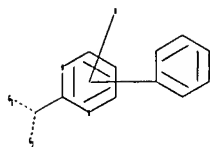


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Uploading C:\Program Files\Stnexp\Queries\10564013.str



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chain nodes :
17 19 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
ring/chain nodes :
13
chain bonds :
3-17 17-19 17-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
17-19 17-21
exact bonds :
3-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 7 :

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G1:O,Cl,Br,F,I

G2:O,N

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 15:Atom 16:Atom 17:CLASS 19:CLASS 21:CLASS

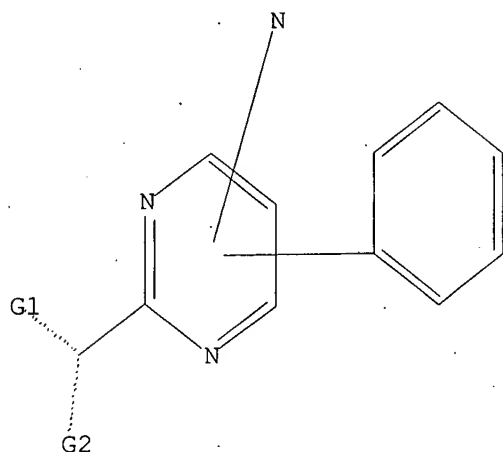
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L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O, Cl, Br, F, I

G2 O, N

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 23:02:38 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1415 TO ITERATE

100.0% PROCESSED 1415 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 26044 TO 30556

PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> => s l1 sss ful

FULL SEARCH INITIATED 23:03:31 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 29728 TO ITERATE

100.0% PROCESSED 29728 ITERATIONS

69 ANSWERS

SEARCH TIME: 00.00.01

L3 69 SEA SSS FUL L1

=> => s l3

L4 8 L3

=> d l4 1-8 bib,ab,hitstr

L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2007:354856 CAPLUS
 DN 146:380000
 TI Preparation of substituted 2-hydroxylaminopyrimidines as agricultural fungicides
 IN Rheinheimer, Joachim; Grote, Thomas; Mueller, Bernd; Lohmann, Jan Klaas; Grammenos, Wassilios; Huenger, Udo; Schieweck, Frank; Ulmschneider, Sarah; Dietz, Jochen; Renner, Jens; Speakman, John-Bryan; Scherer, Maria; Strathmann, Siegfried; Stierl, Reinhard
 PA BASF A.-G., Germany
 SO Ger. Offen., 89pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

Common Inv.

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI.	DE 102005046592	A1	20070329	DE 2005-102005046592	20050928
	WO 2007036477	A1	20070405	WO 2006-EP66572	20060921

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI DE 2005-102005046592 A 20050928

OS MARPAT 146:380000

AB Title compds. [I; R1, R2 = H, (halo)alkyl, (halo)alkenyl, (halo)alkynyl, (halo)cycloalkyl, etc. or R1NOR2 = 5-7 membered (saturated) (substituted) heterocyclyl; R3 = halo, cyano, azido, (substituted) (halo)alkyl, (halo)alkenyl, (halo)alkynyl, etc.; R4 = 5-6 membered (saturated) aromatic (substituted) heterocyclyl containing O, N and S; B = Ph, 5-6 membered heteroaryl containing O, N and S; L = halo, cyano, OCN, (halo)alkyl, (halo)alkenyl, (halo)alkynyl, etc.; n = 1-5], were prepared Thus, 95% NaH in THF was stirred with 1,2,4-triazole for 3 h at room temperature followed by stirring with 4-chloro-2-methylsulfonyl-6-(6-methyltetrahydro-2H-1,2-oxazin-2-yl)-5-(2,4,6-trifluorophenyl)pyrimidine (preparation given) over night at room temperature to give

4-chloro-6-(6-methyltetrahydro-2H-1,2-oxazin-2-yl)-2-(1,2,4-triazol-1-yl)-5-(2,4,6-trifluorophenyl)pyrimidine. The latter as a 250 ppm spray on tomato leaves infected with *Alternaria solani* reduced the infection to 20%, vs. 90% for untreated controls.

IT 931118-01-3P 931118-17-1P 931118-20-6P
 931118-31-9P

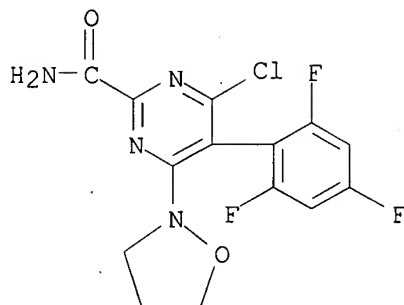
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted hydroxylaminopyrimidines as agricultural fungicides)

RN 931118-01-3 CAPLUS

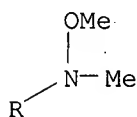
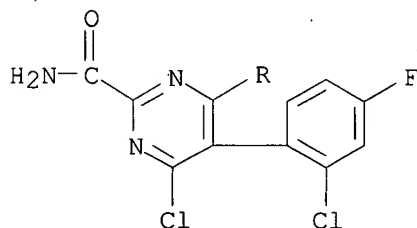
CN 2-Pyrimidinecarboxamide, 4-chloro-6-(2-isoxazolidinyl)-5-(2,4,6-trifluorophenyl)- (CA INDEX NAME)

no pending US appl.



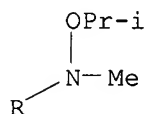
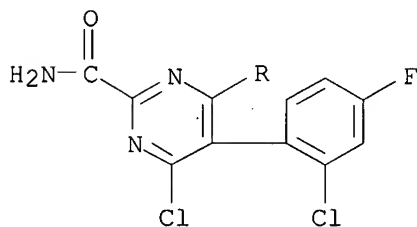
RN 931118-17-1 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-(methoxymethylamino)- (CA INDEX NAME)



RN 931118-20-6 CAPLUS

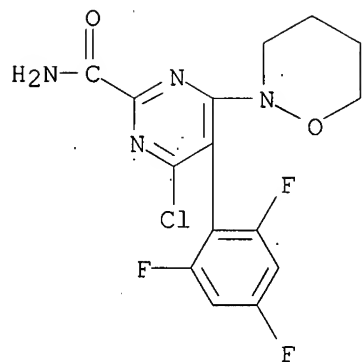
CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[methyl (1-methylethoxy) amino]- (CA INDEX NAME)



RN 931118-31-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-(tetrahydro-2H-1,2-oxazin-2-yl)-5-(2,4,6-trifluorophenyl)- (CA INDEX NAME)

10/564,013



L4 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2006:768723 CAPLUS
 DN 145:180954
 TI Substituted 5-phenylpyrimidines for use in cancer therapy
 IN Rheinheimer, Joachim; Grote, Thomas; Mueller, Bernd; Nave, Barbara;
 Schieweck, Frank; Schwoegler, Anja; Jabs, Thorsten; Blettner, Carsten
 PA BASF Aktiengesellschaft, Germany
 SO PCT Int. Appl., 60pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

Common In

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006079556	A2	20060803	WO 2006-EP774	20060130
	WO 2006079556	A3	20060921		
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RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRAI EP 2005-1955 A 20050131

no pending US appl.

OS MARPAT 145:180954

AB The invention discloses substituted 5-phenylpyrimidines I [X = NR₁R₂, OR_{1a}, SR_{1a}, (R₁, R₂ = H, C₁-C₁₀ alkyl, C₂-C₆-alkenyl, etc.; R_{1a} = R₁ except for hydrogen); Y = halo, cyano, C₁-C₄-alkyl, etc.; R₄ = radical of 1-15 atoms different from H; L = radical of 1-10 atoms different from H; n = 0-5], or a pharmaceutically acceptable salt thereof, for use in therapy, in particular for the therapy of cancerous diseases.

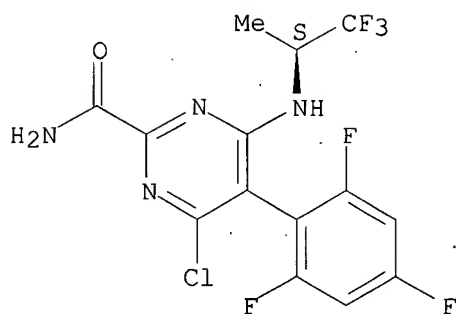
IT 838838-62-3 838838-71-4 838838-82-7
 838838-84-9 838838-88-3 838838-89-4
 903549-09-7 903549-10-0 903549-20-2
 903549-35-9

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (phenylpyrimidine derivs. for cancer therapy)

RN 838838-62-3 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

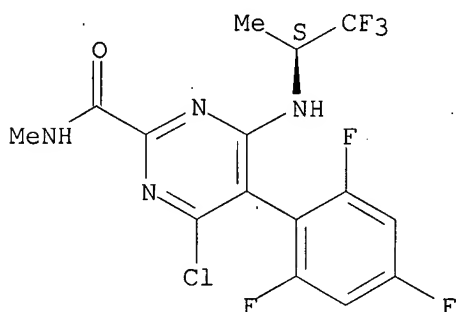
Absolute stereochemistry.



RN 838838-71-4 CAPLUS

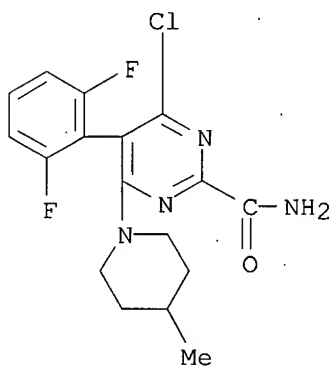
CN 2-Pyrimidinecarboxamide, 4-chloro-N-methyl-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 838838-82-7 CAPLUS

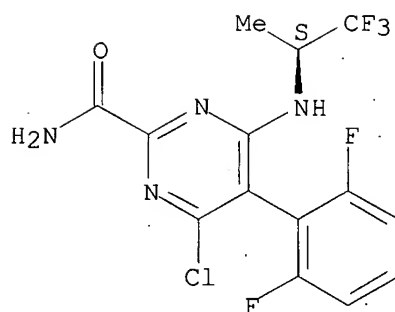
CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 838838-84-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluorophenyl)-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]- (9CI) (CA INDEX NAME)

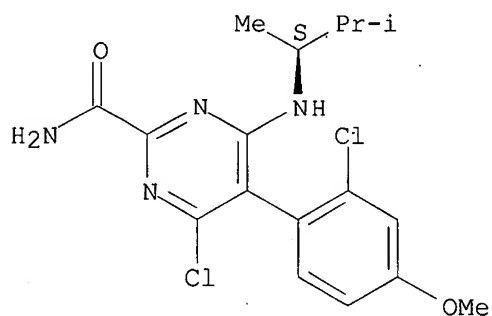
Absolute stereochemistry.



RN 838838-88-3 CAPLUS

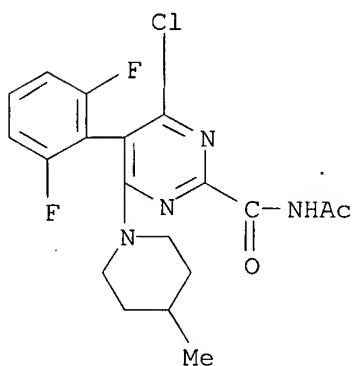
CN 2-Pyrimidinecarboxamide, 4-chloro-5-((1S)-1,2-dimethylpropyl)amino]-6-[[(1S)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



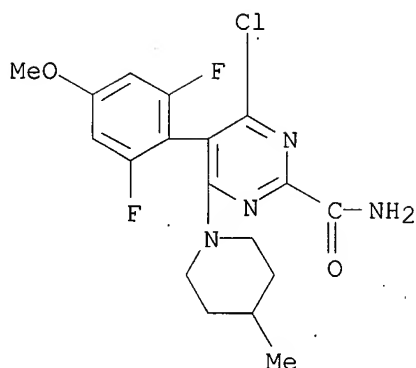
RN 838838-89-4 CAPLUS

CN 2-Pyrimidinecarboxamide, N-acetyl-4-chloro-5-((1S)-1,2-dimethylpropyl)amino-6-(2-chloro-4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 903549-09-7 CAPLUS

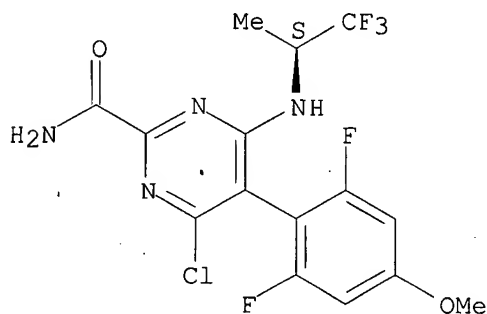
CN 2-Pyrimidinecarboxamide, 4-chloro-5-((1S)-1,2-dimethylpropyl)amino-6-(2,6-difluorophenyl)- (9CI) (CA INDEX NAME)



RN 903549-10-0 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluoro-4-methoxyphenyl)-6-
[[1S)-2,2,2-trifluoro-1-methylethyl]amino]- (9CI) (CA INDEX NAME)

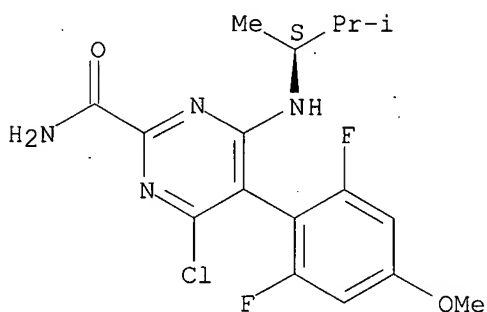
Absolute stereochemistry.



RN 903549-20-2 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluoro-4-methoxyphenyl)-6-
[[1S)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

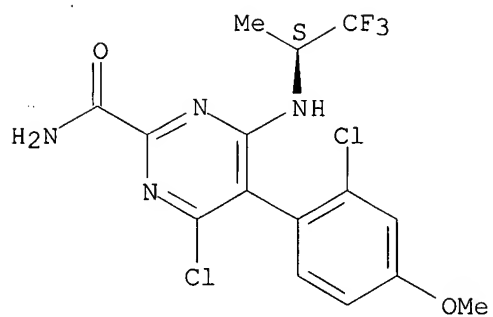


RN 903549-35-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-methoxyphenyl)-6-[[1S)-
2,2,2-trifluoro-1-methylethyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/564,013



L4 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2005:120896 CAPLUS
 DN 142:198096
 TI Preparation of 2-acyl-4-amino-5-arylpyrimidines as pesticides and fungicides.
 IN Schwoegler, Anja; Gewehr, Markus; Mueller, Bernd; Grote, Thomas; Grammenos, Wassilios; Tormo I. Blasco, Jordi; Gypser, Andreas; Rheinheimer, Joachim; Blettner, Carsten; Schaefer, Peter; Schieweck, Frank; Wagner, Oliver; Stierl, Reinhard; Schoefl, Ulrich; Strathmann, Siegfried; Scherer, Maria
 PA BASF Aktiengesellschaft, Germany
 SO PCT Int. Appl., 79 pp.
 CODEN: PIXXD2

DT Patent
 LA German

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005012261	A1	20050210	WO 2004-EP7877	20040715
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004261373	A1	20050210	AU 2004-261373	20040715
	CA 2532718	A1	20050210	CA 2004-2532718	20040715
	EP 1651618	A1	20060503	EP 2004-741053	20040715
	EP 1651618	B1	20070103		
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	CN 1829700	A	20060906	CN 2004-80021440	20040715
	BR 2004012891	A	20061003	BR 2004-12891	20040715
	JP 2006528603	T	20061221	JP 2006-520743	20040715
	AT 350370	T	20070115	AT 2004-741053	20040715
	MX 2006PA00038	A	20060321	MX 2006-PA38	20060105
	IN 2006CN00644	A	20070608	IN 2006-CN644	20060222
	US 2007105873	A1	20070510	US 2007-564013	20070109
PRAI	DE 2003-10333857	A	20030724		
	DE 2003-10357714	A	20031209		
	WO 2004-EP7877	W	20040715		

OS MARPAT 142:198096

AB Title compds. [I; n = 1-5; L = halo, cyano, cyanato, alkyl, alkenyl, alkynyl, alkoxy, alkenyloxy, alkynyloxy, cycloalkyl, cycloalkoxy, etc.; R1, R2 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, halocycloalkyl; R1R2N = atoms to form 5-6 membered (substituted) heterocyclyl; R3 = halo, cyano, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, alkenyloxy, alkynyloxy, alkylthio, etc.; R4 = CONHXRa, C(ORb):NXRa; X = bond, CO, CONH, CO2, O, imino, etc.; Ra = H, alkyl, alkenyl, alkynyl, PhCH2; Rb = H, alkyl, alkenyl, alkynyl], were prepared Thus, (S)-4-chloro-6-(2,2,2-trifluoro-1-methylethylamino)-5-(2,4,6-trifluorophenyl)pyrimidine-2-carbonitrile was stirred with K2CO3 and H2O2 in Me2SO at 10°-room temperature to give (S)-4-chloro-6-(2,2,2-trifluoro-1-methylethylamino)-5-(2,4,6-trifluorophenyl)pyrimidine-2-carboxamide. The latter at 250 ppm on tomatoes gave complete protection against

Phytophthora infestans.

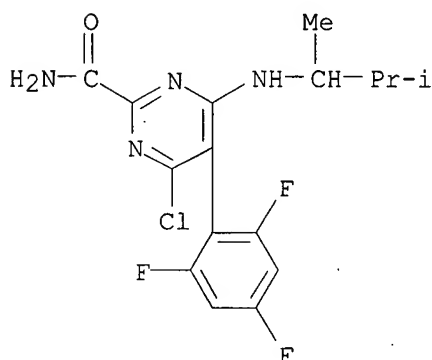
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 838839-12-6P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of acylaminoarylpyrimidines as pesticides and fungicides)

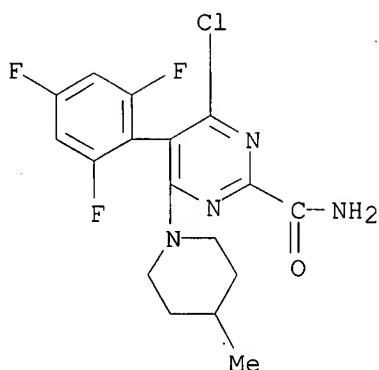
RN 838838-58-7 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-[(1,2-dimethylpropyl)amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)



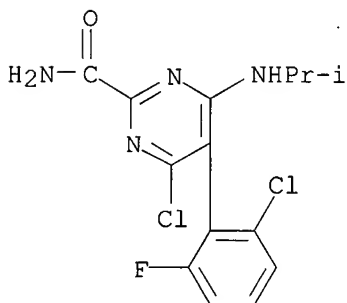
RN 838838-59-8 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-(4-methyl-1-piperidinyl)-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)



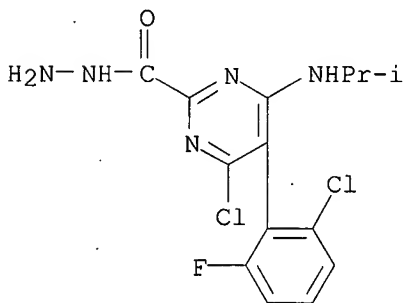
RN 838838-60-1 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-6-fluorophenyl)-6-[(1-methylethyl)amino]- (9CI) (CA INDEX NAME)



RN 838838-61-2 CAPLUS

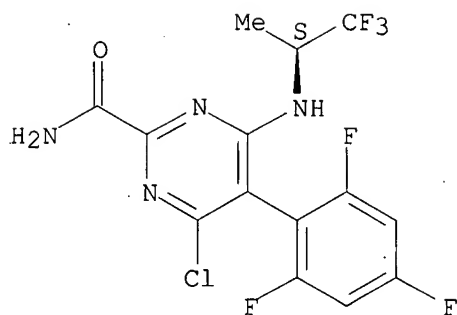
CN 2-Pyrimidinecarboxylic acid, 4-chloro-5-(2-chloro-6-fluorophenyl)-6-[(1-methylethyl)amino]-, hydrazide (9CI) (CA INDEX NAME)



RN 838838-62-3 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

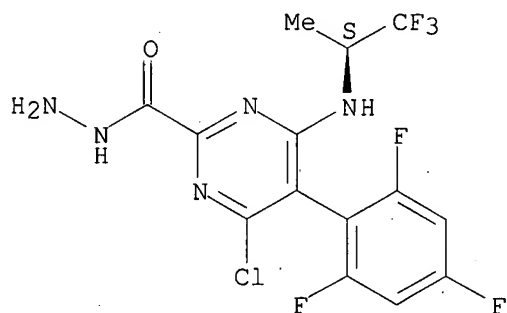
Absolute stereochemistry.



RN 838838-63-4 CAPLUS

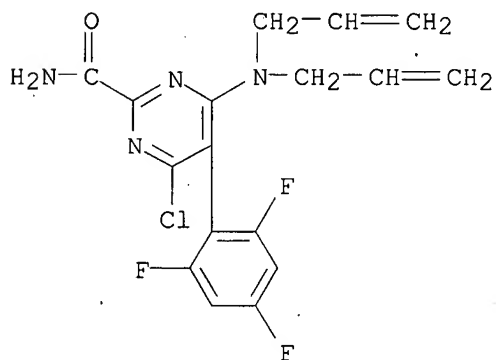
CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



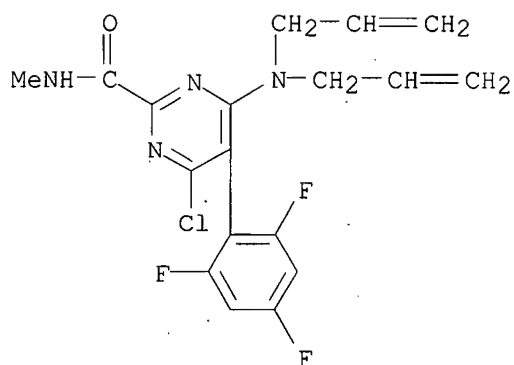
RN 838838-64-5 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-(di-2-propenylamino)-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)



RN 838838-65-6 CAPLUS

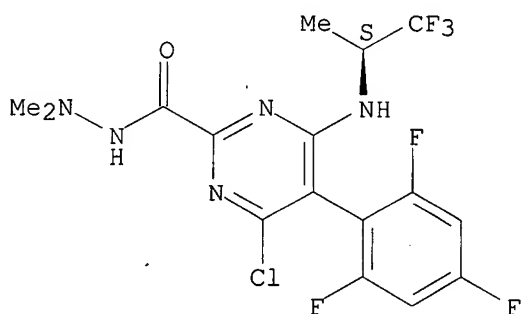
CN 2-Pyrimidinecarboxamide, 4-chloro-6-(di-2-propenylamino)-N-methyl-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)



RN 838838-66-7 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2,2-dimethylhydrazide (9CI)
(CA INDEX NAME)

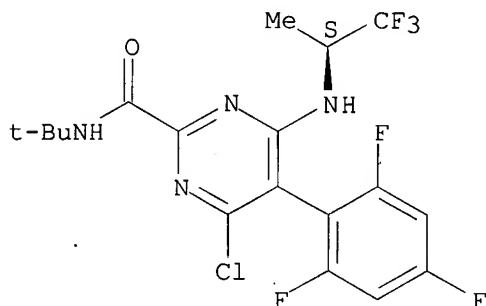
Absolute stereochemistry.



RN 838838-67-8 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-N-(1,1-dimethylethyl)-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

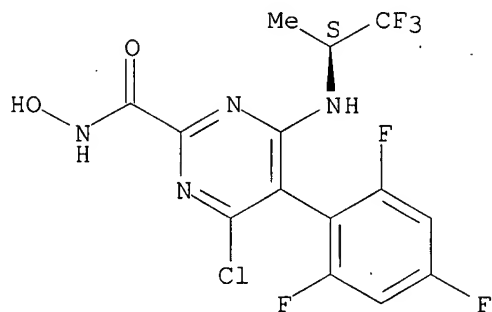
Absolute stereochemistry.



RN 838838-68-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-N-hydroxy-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

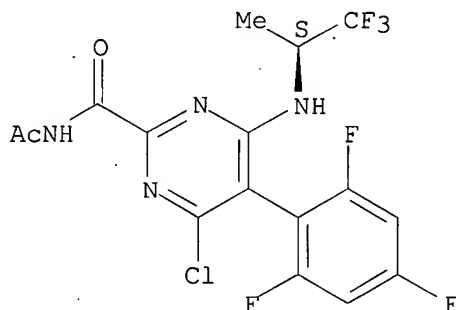
Absolute stereochemistry.



RN 838838-69-0 CAPLUS

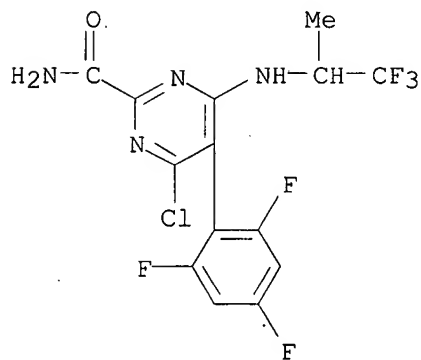
CN 2-Pyrimidinecarboxamide, N-acetyl-4-chloro-6-[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 838838-70-3 CAPLUS

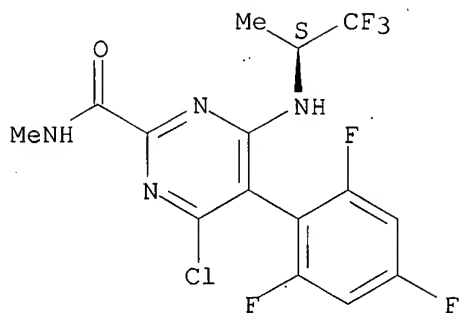
CN 2-Pyrimidinecarboxamide, 4-chloro-6-[(2,2,2-trifluoro-1-methylethyl)amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)



RN 838838-71-4 CAPLUS

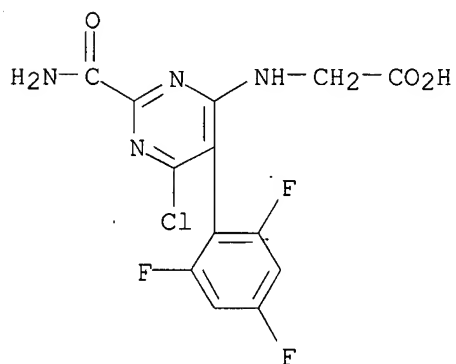
CN 2-Pyrimidinecarboxamide, 4-chloro-N-methyl-6-[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 838838-72-5 CAPLUS

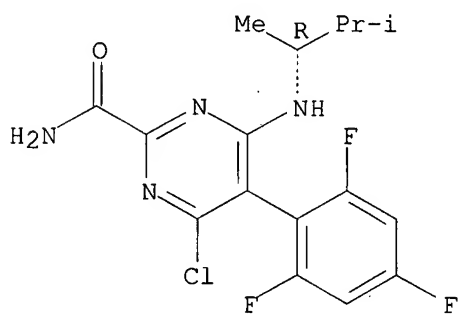
CN Glycine, N-[2-(aminocarbonyl)-6-chloro-5-(2,4,6-trifluorophenyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 838838-73-6 CAPLUS

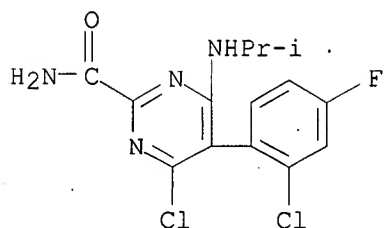
CN 2-Pyrimidinecarboxamide, 4-chloro-6-[[(1R)-1,2-dimethylpropyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



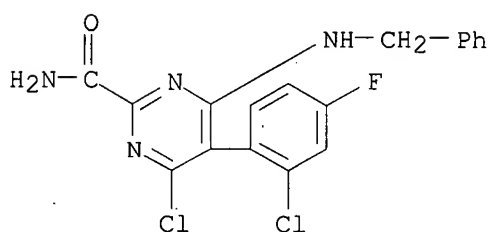
RN 838838-74-7 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[(1-methylethyl)amino]- (9CI) (CA INDEX NAME)



RN 838838-75-8 CAPLUS

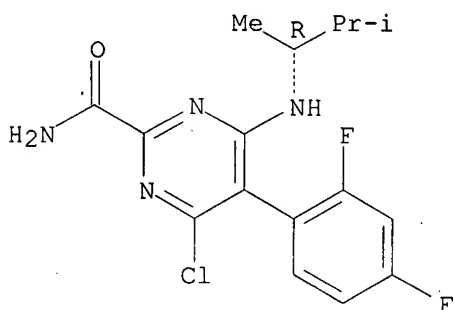
CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 838838-76-9 CAPLUS

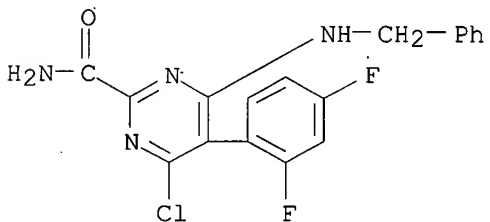
CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-[(1R)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 838838-77-0 CAPLUS

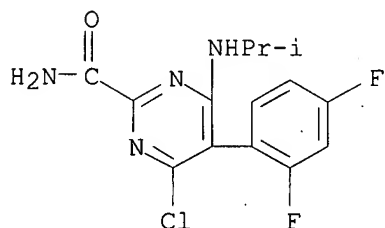
CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



10/564,013

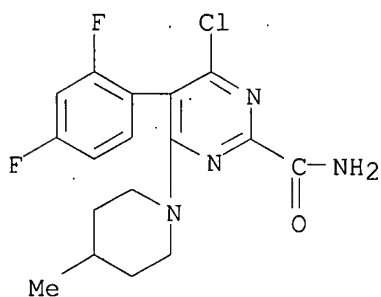
RN 838838-78-1 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-[(1-methylethyl)amino]- (9CI) (CA INDEX NAME)



RN 838838-79-2 CAPLUS

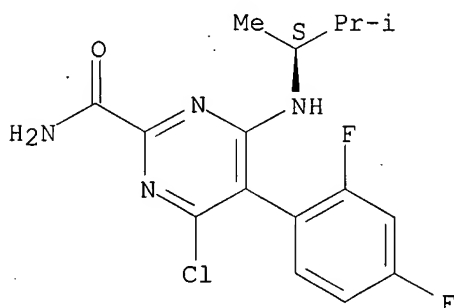
CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-(4-methyl-1-piperidiny)- (9CI) (CA INDEX NAME)



RN 838838-80-5 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-[[(1S)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

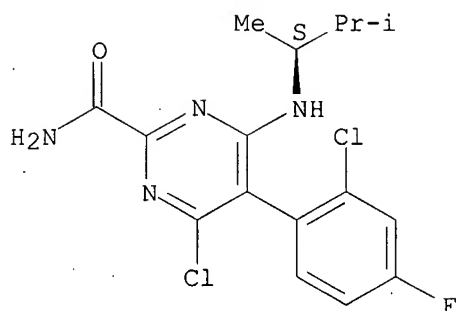
Absolute stereochemistry.



RN 838838-81-6 CAPLUS

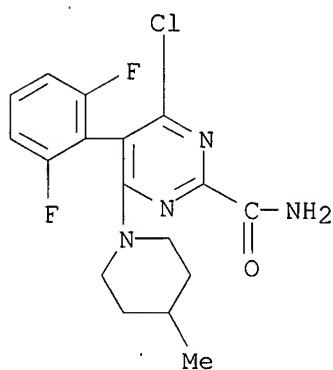
CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[[(1S)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



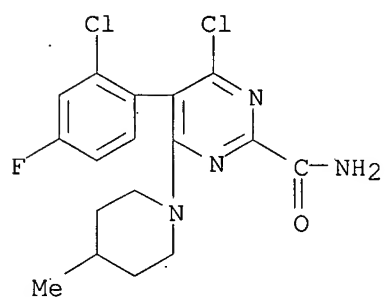
RN 838838-82-7 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 838838-83-8 CAPLUS

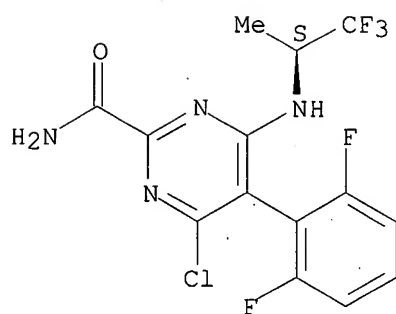
CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 838838-84-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluorophenyl)-6-[(1S)-2,2,2-trifluoro-1-methylethylamino]- (9CI) (CA INDEX NAME)

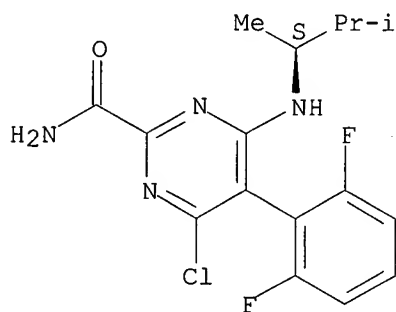
Absolute stereochemistry.



RN 838838-85-0 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluorophenyl)-6-[[(1S)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

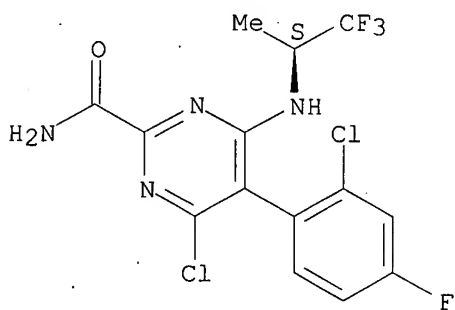
Absolute stereochemistry.



RN 838838-86-1 CAPLUS

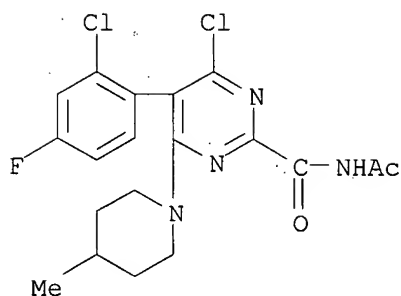
CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 838838-87-2 CAPLUS

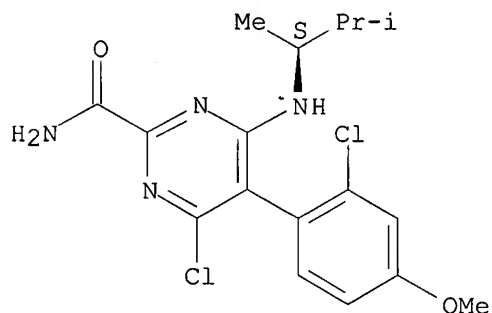
CN 2-Pyrimidinecarboxamide, N-acetyl-4-chloro-5-(2-chloro-4-fluorophenyl)-6-(4-methyl-1-piperidiny)- (9CI) (CA INDEX NAME)



RN 838838-88-3 CAPLUS

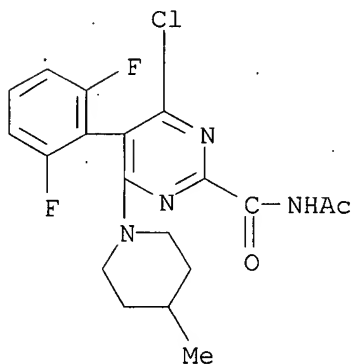
CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-methoxyphenyl)-6-[[1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 838838-89-4 CAPLUS

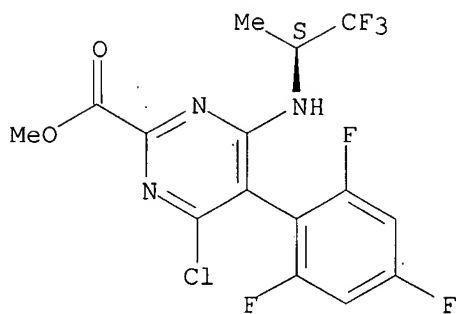
CN 2-Pyrimidinecarboxamide, N-acetyl-4-chloro-5-(2,6-difluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)



RN 838838-90-7 CAPLUS

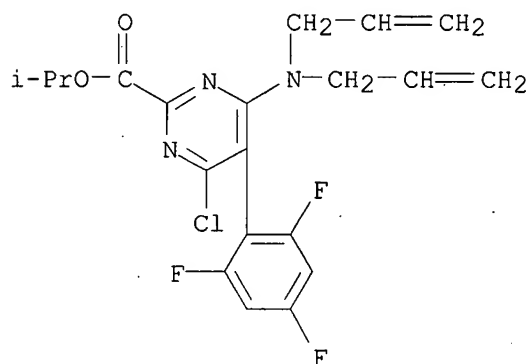
CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[1,2,2,2-tetrafluoroethyl]amino]-5-(2,4,6-trifluorophenyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 838838-91-8 CAPLUS

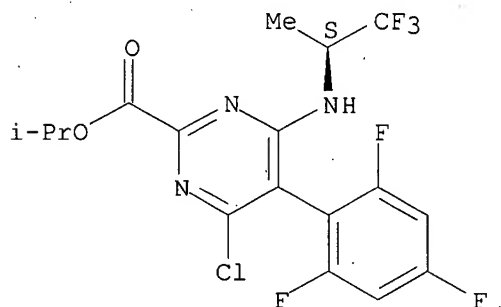
CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-((1S)-2,2,2-trifluoro-1-methylethylamino)-5-(2,4,6-trifluorophenyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 838838-92-9 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)

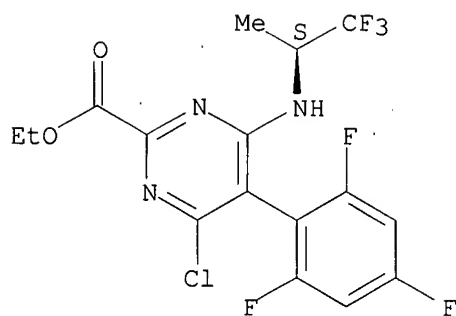
Absolute stereochemistry.



RN 838838-93-0 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, ethyl ester (9CI) (CA INDEX NAME)

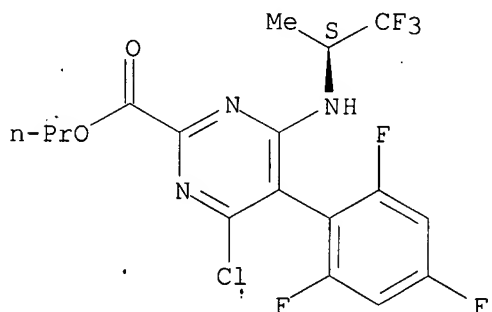
Absolute stereochemistry.



RN 838838-94-1 CAPLUS

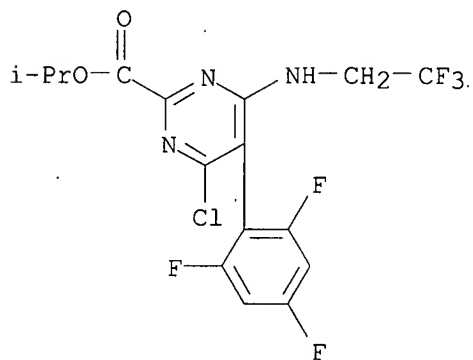
CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 838838-95-2 CAPLUS

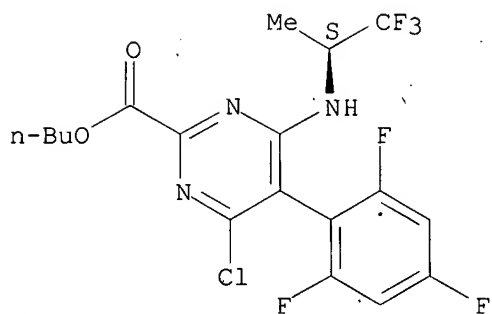
CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[(2,2,2-trifluoroethyl)amino]-5-(2,4,6-trifluorophenyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 838838-96-3 CAPLUS

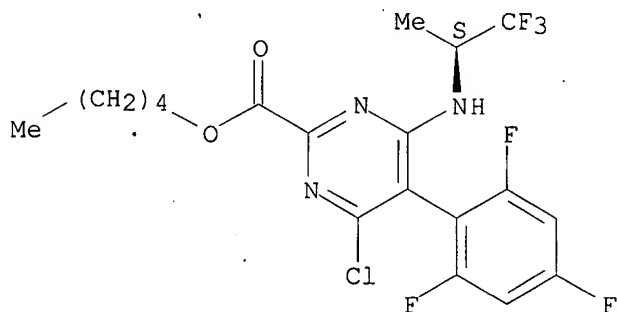
CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, butyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



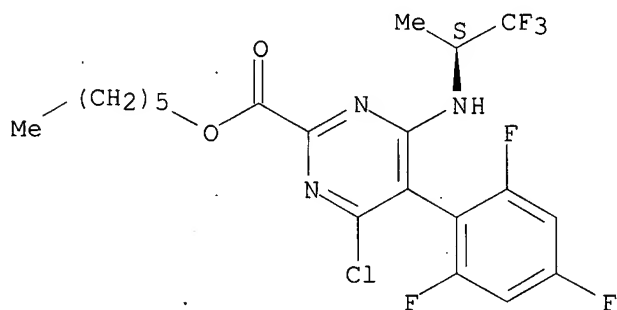
RN 838838-97-4 CAPLUS
 CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, pentyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



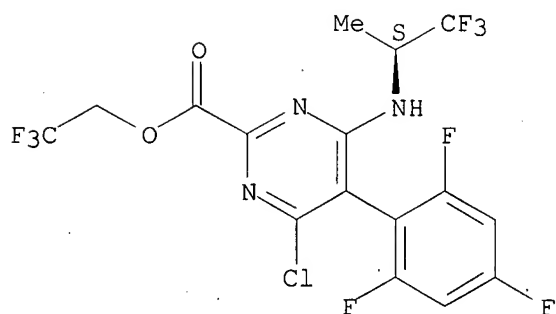
RN 838838-98-5 CAPLUS
 CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, hexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



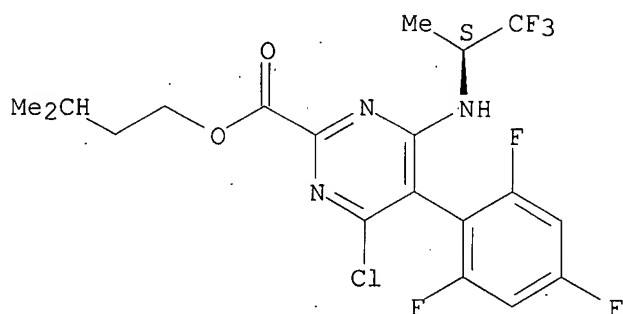
RN 838838-99-6 CAPLUS
 CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2,2,2-trifluoroethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



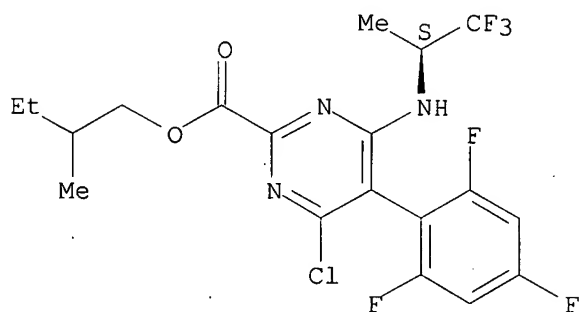
RN 838839-00-2 CAPLUS
 CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 3-methylbutyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



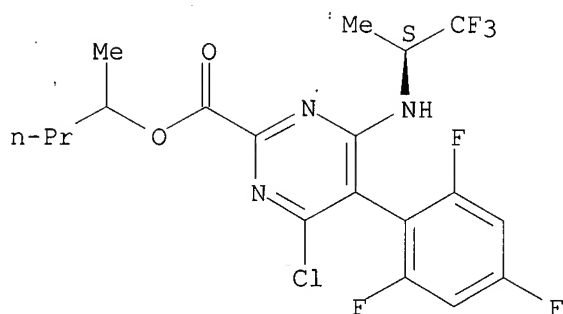
RN 838839-01-3 CAPLUS
 CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2-methylbutyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



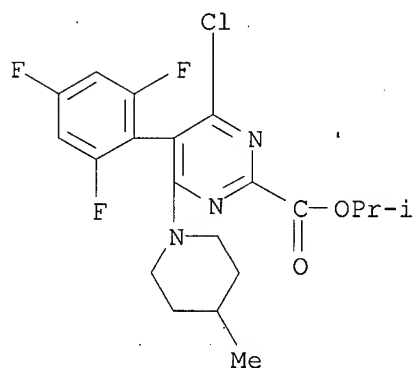
RN 838839-02-4 CAPLUS
 CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 1-methylbutyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 838839-03-5 CAPLUS

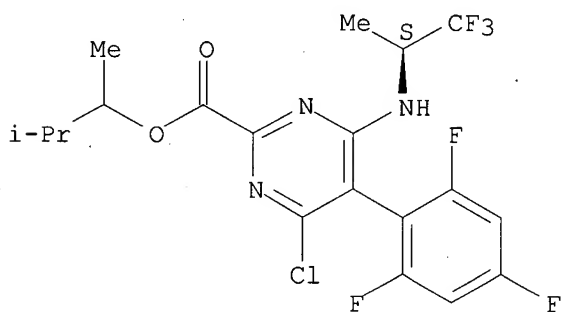
CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-(4-methyl-1-piperidinyl)-5-(2,4,6-trifluorophenyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 838839-04-6 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[(1S)-2,2,2-trifluoro-1-methylethylamino]-5-(2,4,6-trifluorophenyl)-, 1,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

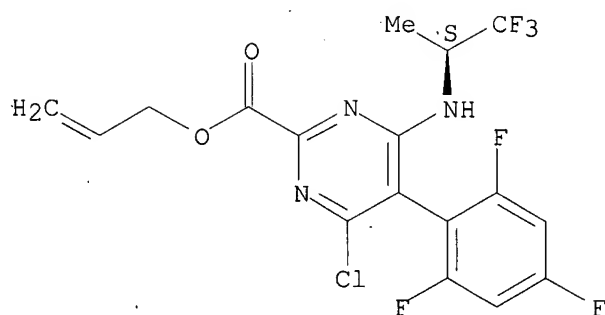
Absolute stereochemistry.



RN 838839-05-7 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[(1S)-2,2,2-trifluoro-1-methylethylamino]-5-(2,4,6-trifluorophenyl)-, 2-propenyl ester (9CI) (CA INDEX NAME)

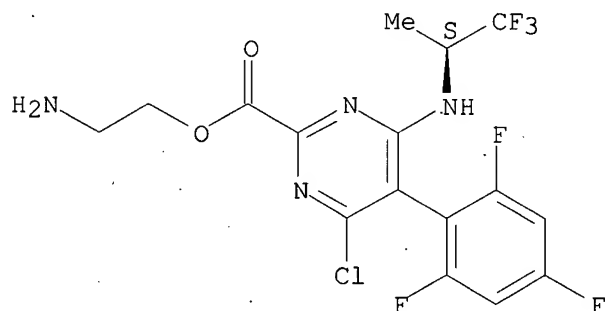
Absolute stereochemistry.



RN 838839-06-8 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2-aminoethyl ester (9CI)
(CA INDEX NAME)

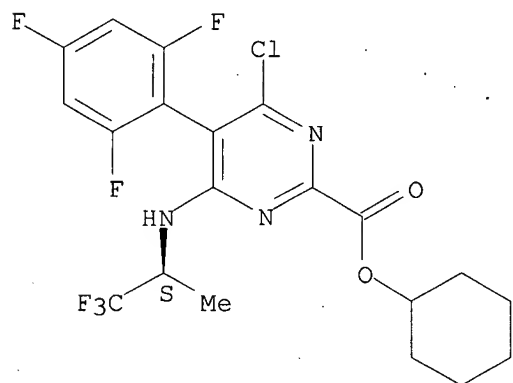
Absolute stereochemistry.



RN 838839-07-9 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, cyclohexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

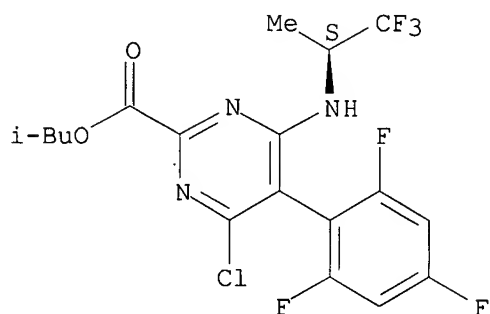


RN 838839-08-0 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2-methylpropyl ester (9CI)

(CA INDEX NAME)

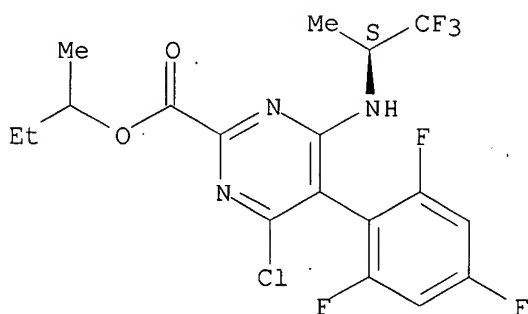
Absolute stereochemistry.



RN 838839-09-1 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 1-methylpropyl ester (9CI)
(CA INDEX NAME)

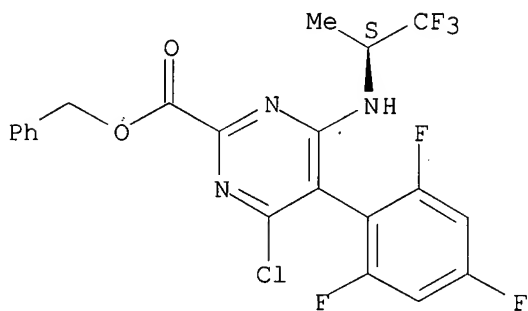
Absolute stereochemistry.



RN 838839-10-4 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, phenylmethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

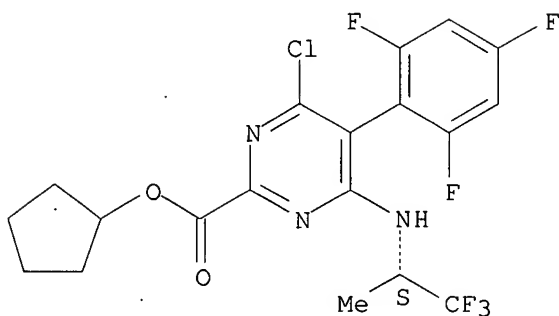


RN 838839-11-5 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, cyclopentyl ester (9CI)

(CA INDEX NAME)

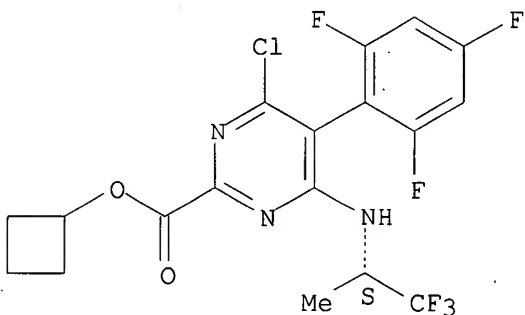
Absolute stereochemistry.



RN 838839-12-6 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, cyclobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



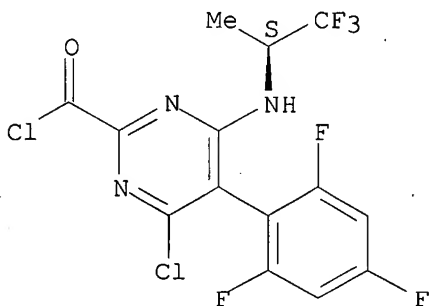
IT 838839-13-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of acylaminoarylpyrimidines as pesticides and fungicides)

RN 838839-13-7 CAPLUS

CN 2-Pyrimidinecarbonyl chloride, 4-chloro-6-[[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2004:817651 CAPLUS
 DN 141:332206
 TI Preparation of biaryl substituted 6-membered heterocycles as sodium channel blockers
 IN Chakravarty, Prasun K.; Fisher, Michael H.; Parsons, William H.; Liang, Jun; Zhou, Bishan
 PA Merck & Co., Inc., USA
 SO PCT Int. Appl., 125 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004084824	A2	20041007	WO 2004-US8532	20040319
WO 2004084824	A3	20050331		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004224392	A1	20041007	AU 2004-224392	20040319
CA 2519677	A1	20041007	CA 2004-2519677	20040319
EP 1608622	A2	20051228	EP 2004-757920	20040319
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1791580	A	20060621	CN 2004-80013599	20040319
JP 2006521357	T	20060921	JP 2006-507395	20040319
US 2006293339	A1	20061228	US 2005-550641	20050923
PRAI US 2003-456312P	P	20030324		
WO 2004-US8532	A	20040319		

OS MARPAT 141:332206

AB The title biaryl substituted pyridine, pyrimidine and pyrazine compds. [I or II; H-1 = (un)substituted pyridyl, pyrimidyl, pyrazinyl; H-2 = (un)substituted pyridyl, pyrimidyl, pyrazinyl; R4, R5 = H, alkyl, alkoxy, aryloxy, etc.; R6-R8 = H, alkyl, cycloalkyl, alkoxy, etc.] which are sodium channel blockers useful for the treatment of pain (no data), were prepared E.g., a 2-step synthesis of III, starting from 2-bromo-6-methylpyridine and 3-bromophenylboronic acid, was given. Claimed pharmaceutical compns. comprise an effective amount of the instant compds. I, either alone, or in combination with one or more therapeutically active compds., and a pharmaceutically acceptable carrier. Methods of treating conditions associated with, or caused by, sodium channel activity, including, for example, acute pain, chronic pain, visceral pain, inflammatory pain, neuropathic pain, epilepsy, irritable bowel syndrome, depression, anxiety, multiple sclerosis, and bipolar disorder, comprise administering an effective amount of the present compds., either alone, or in combination with one or more other therapeutically active compds.

IT 770727-12-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

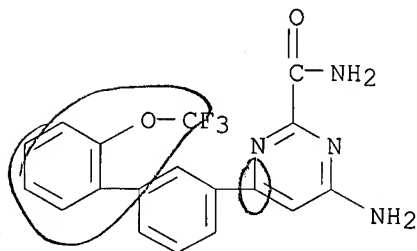
(preparation of biaryl substituted 6-membered heterocycles as sodium channel

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blockers for treatment or prevention of pain)

RN 770727-12-3 CAPLUS

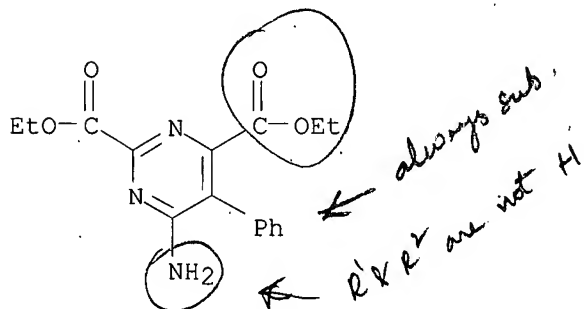
CN 2-Pyrimidinecarboxamide, 4-amino-6-[2'-(trifluoromethoxy)[1,1'-biphenyl]-3-yl]- (9CI) (CA INDEX NAME)



2 dybb
L is not phenyl

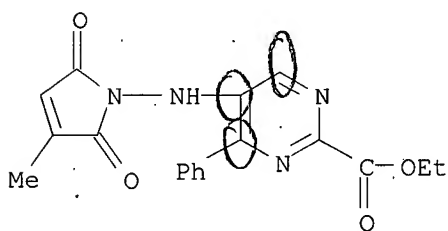
✓

L4 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2004:205964 CAPLUS
 DN 142:74474
 TI Product class 12: pyrimidines
 AU von Angerer, S.
 CS Germany
 SO Science of Synthesis (2004), 16, 379-572
 CODEN: SSCYJ9
 PB Georg Thieme Verlag
 DT Journal; General Review
 LA English
 AB A review. Methods for preparing pyrimidines are reviewed including cyclization, ring transformation, aromatization and substituent modification.
 IT 157201-09-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of pyrimidines via cyclization, ring transformation, aromatization and substituent modification)
 RN 157201-09-7 CAPLUS
 CN 2,4-Pyrimidinedicarboxylic acid, 6-amino-5-phenyl-, diethyl ester (9CI)
 (CA INDEX NAME)



RE.CNT 856 THERE ARE 856 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

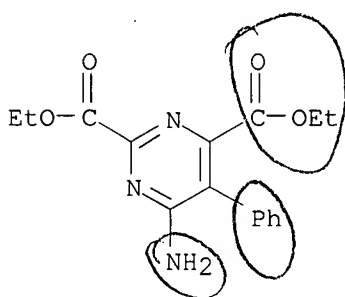
L4 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2003:385500 CAPLUS
 DN 139:111073
 TI QSAR Study of Ethyl 2-[(3-Methyl-2,5-dioxo(3-pyrrolinyl))amino]-4-(trifluoromethyl) pyrimidine-5-carboxylate: An Inhibitor of AP-1 and NF- κ B Mediated Gene Expression Based on Support Vector Machines
 AU Liu, H. X.; Zhang, R. S.; Yao, X. J.; Liu, M. C.; Hu, Z. D.; Fan, B. T.
 CS Department of Chemistry, Department of Computer Science and State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou, 730000, Peop. Rep. China
 SO Journal of Chemical Information and Computer Sciences (2003), 43(4), 1288-1296
 CODEN: JCISD8; ISSN: 0095-2338
 PB American Chemical Society
 DT Journal
 LA English
 AB The support vector machine, as a novel type of learning machine, for the first time, was used to develop a QSAR model of 57 analogs of Et 2-[(3-methyl-2,5-dioxo(3-pyrrolinyl))amino]-4-(trifluoromethyl)pyrimidine-5-carboxylate (EPC), an inhibitor of AP-1 and NF- κ B mediated gene expression, based on calculated quantum chemical parameters. The quantum chemical parameters involved in the model are Kier and Hall index (order 3) (KHI3), Information content (order 0) (IC0), YZ Shadow (YZS) and Max partial charge for an N atom (MaxPCN), Min partial charge for an N atom (MinPCN). The mean relative error of the training set, the validation set, and the testing set is 1.35%, 1.52%, and 2.23%, resp., and the maximum relative error is less than 5.00%.
 IT 561322-59-6
 RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
 (QSAR study of Et pyrimidinecarboxylates, inhibitor of AP-1 and NF- κ B mediated gene expression based on support vector machines)
 RN 561322-59-6 CAPLUS
 CN 2-Pyrimidinecarboxylic acid, 5-[(2,5-dihydro-3-methyl-2,5-dioxo-1H-pyrrol-1-yl)amino]-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



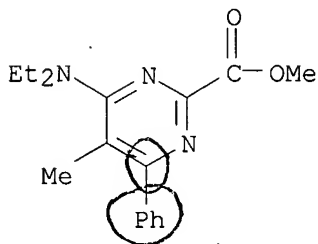
R^3 is Not H
 both positions are different.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 1994:534077 CAPLUS
 DN 121:134077
 TI Inverse Electron Demand Diels-Alder Reactions of Heterocyclic Azadienes:
 [4 + 2] Cycloaddition Reaction of Amidines with 1,3,5-Triazines
 AU Boger, Dale L.; Kochanny, Monica J.
 CS Department of Chemistry, Scripps Research Institute, La Jolla, CA, 92037,
 USA
 SO Journal of Organic Chemistry (1994), 59(17), 4950-5
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 OS CASREACT 121:134077
 AB A detailed study of the scope of the amidine I (R = H, alkyl, etc.; X =
 NH₂CH₂CH₂NH, etc.) Diels-Alder reaction with 1,3,5-triazines II (R = H,
 EtO₂C, MeS) is described. The thermal reaction of amidines with sym.
 1,3,5-triazines proceeds with in situ amidine to 1,1-diaminoethene
 tautomerization, [4+2] cycloaddn. with the 1,3,5-triazine, loss of ammonia
 from the initial Diels-Alder adduct with imine generation, imine to
 enamine tautomerization, and retro Diels-Alder loss of Et cyanoformate to
 provide substituted 4-aminopyrimidines in excellent conversions. The
 reaction proceeds best with the amidine hydrochloride salts at
 intermediate reaction temps. (90-100 °C) in polar, aprotic
 solvents, is rather invariant to the ratio of dienophile-diene used (1:2
 equivalent 1:1 equivalent. 2:1), and is subject to triazine substituent effects
 characteristic of an inverse electron demand Diels-Alder reaction (R =
 CO₂Et > R = H » R = SCH₃). Notably, the generality of the amidine
 [4+2] cycloaddn. reaction with 1,3,5-triazines which was extended to
 include cyclic amidines effectively addresses the limitations of the
 alternative ynamine or N,O-ketene acetal dienophiles. A comparative
 examination of amidines, thioimidates, and imidates revealed that amidines are
 uniquely suited for use in this reaction cascade.
 IT 157201-09-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 157201-09-7 CAPLUS
 CN 2,4-Pyrimidinedicarboxylic acid, 6-amino-5-phenyl-, diethyl ester (9CI)
 (CA INDEX NAME)

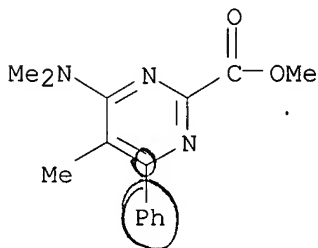


L4 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 1975:579010 CAPLUS
 DN 83:179010
 TI Competing cycloaddition in the reaction of 1,2,4-triazines with ynamines
 AU Reim, H.; Steigel, A.; Sauer, J.
 CS Inst. Chem., Univ. Regensburg, Regensburg, Fed. Rep. Ger.
 SO Tetrahedron Letters (1975), (33), 2901-4
 CODEN: TELEAY; ISSN: 0040-4039
 DT Journal
 LA German
 OS CASREACT 83:179010
 AB The triazines I (R = H, Ph, R1 = H) with MeC.tplbond.CNEt2 gave 100% pyrimidines II by 2,5-addition I (R = H, R1 = Ph), for which 2,5-addition is blocked by Ph, gave 85% pyridine III (R2 = Me, R3 = NEt2) as the only product by 3,6-addition I (R = R1 = CO2Me, Me) gave mixts. of II and III (R2 = Me, R3 = NEt2) and similarly, with PhC.tplbond.CH, gave III (R2 = Ph, R3 = H; R2 = H, R3 = Ph). I (R = R1 = Ph) with MeC.tplbond.CNEt2 gave II and III (R2 = Me, R3 = NEt2; R2 = NEt2, R3 = Me) similar reactions with MeC.tplbond.CNMe2 gave analogous results. The proportions of the mixts. obtained were solvent dependent.
 IT 57767-98-3P 57768-01-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 57767-98-3 CAPLUS
 CN 2-Pyrimidinecarboxylic acid, 4-(diethylamino)-5-methyl-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)



2 diff no activity

RN 57768-01-1 CAPLUS
 CN 2-Pyrimidinecarboxylic acid, 4-(dimethylamino)-5-methyl-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)



10/564,013

=> => d his

(FILE 'HOME' ENTERED AT 23:01:59 ON 02 AUG 2007)

FILE 'REGISTRY' ENTERED AT 23:02:09 ON 02 AUG 2007

L1 STRUCTURE UPLOADED
L2 3 S L1 SSS SAM
L3 69 S L1 SSS FUL

FILE 'CAPLUS' ENTERED AT 23:03:38 ON 02 AUG 2007

L4 8 S L3

FILE 'CAOLD' ENTERED AT 23:04:07 ON 02 AUG 2007

=> s 13

L5 0 L3

=> log y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.45	215.84

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-6.24

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 23:04:20 ON 02 AUG 2007